



Soft X-Ray Spectroscopy with synchrotron radiation as a powerful tool for Materials Research

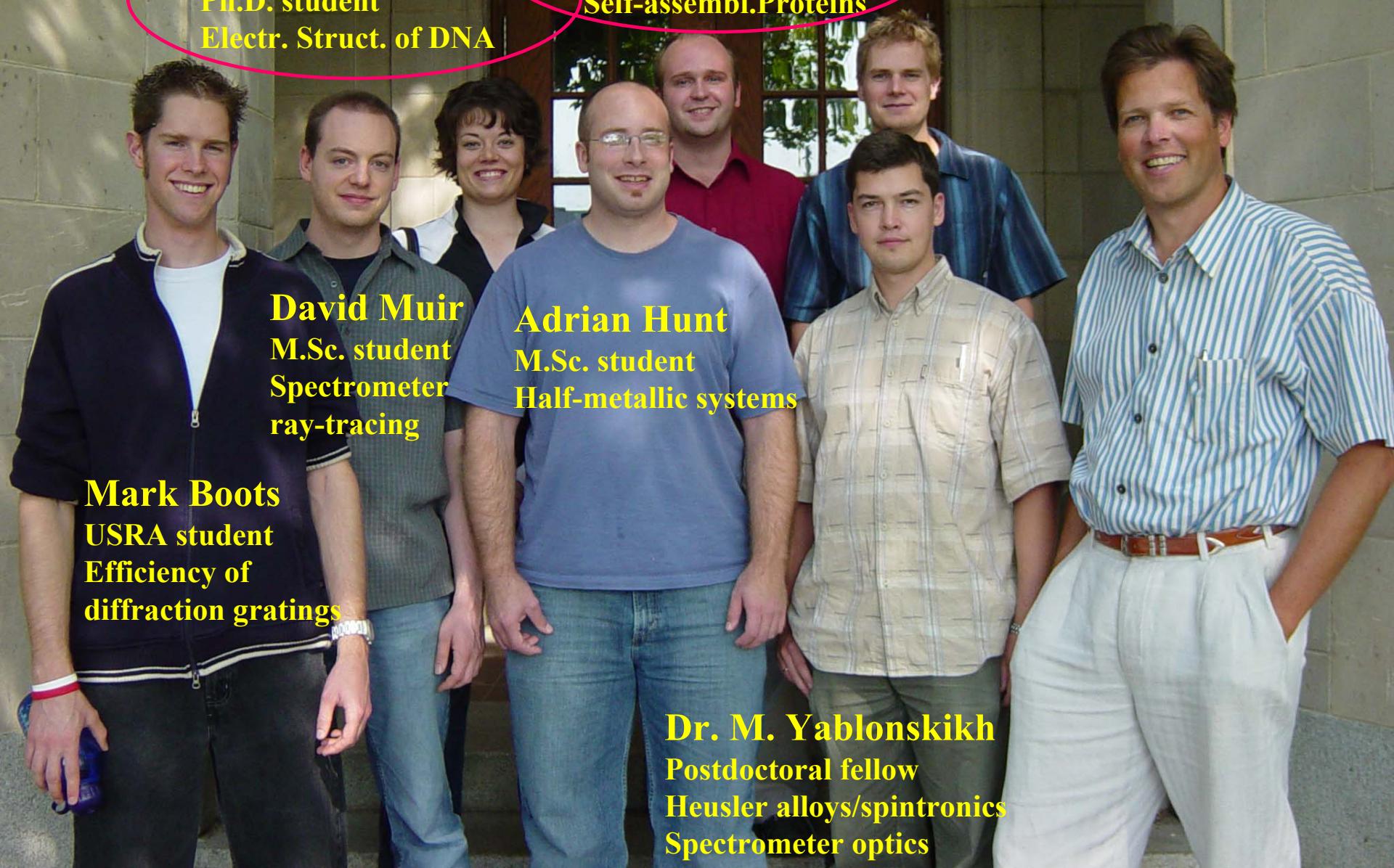
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Frontiers in Photon-in Photon/Photon-out Spectroscopy, Berkeley Oct. 22nd, 2005

The group



Janay MacNaughton
Ph.D. student
Electr. Struct. of DNA

Regan Wilks
Ph.D. student
Self-assembl.Proteins

Tor Pedersen
M.Sc. student
Organic magnetic
devides

Mark Boots
USRA student
Efficiency of
diffraction gratings

David Muir
M.Sc. student
Spectrometer
ray-tracing

Adrian Hunt
M.Sc. student
Half-metallic systems

Dr. M. Yablonskikh
Postdoctoral fellow
Heusler alloys/spintronics
Spectrometer optics

Outline

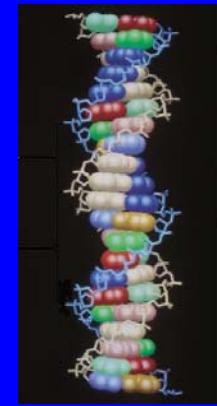
1. What is the conductivity of DNA?
 2. Where do I see future improvements of photon-in photon-out techniques?
 3. Our new soft x-ray emission spectrometer.

What are the questions we are asking ?

- What happens when metal ions are implemented in a host matrix ?

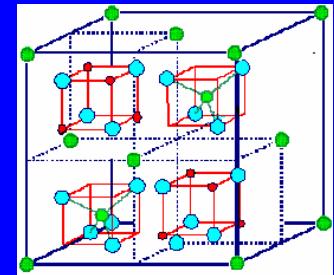


Ion bombarded polymers



(M)-DNA

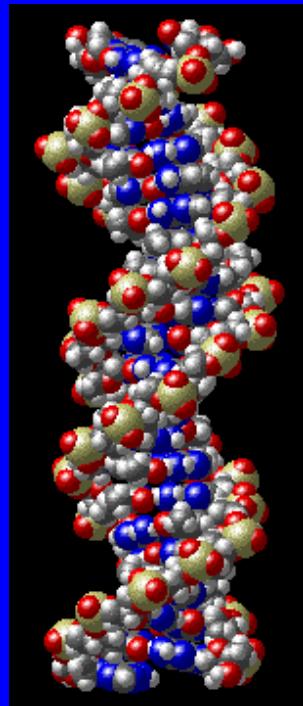
- Can we excite different sites selectively in order to learn more about complex systems ?



$\gamma\text{-Si}_3\text{N}_4$

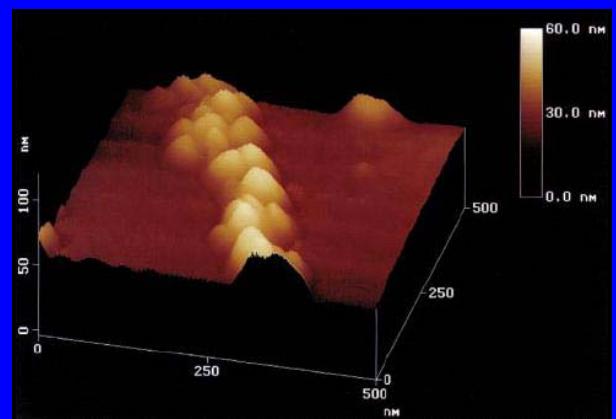
- In general: Can we link spectroscopic (structural) information to functionality ?

Electronic properties of double strand DNA



Why is DNA interesting?

- Can easily synthesize a variety of structures
→ Nanowires
- Self-assembling properties!
- High molecular recognition possibilities
→ biological sensors.

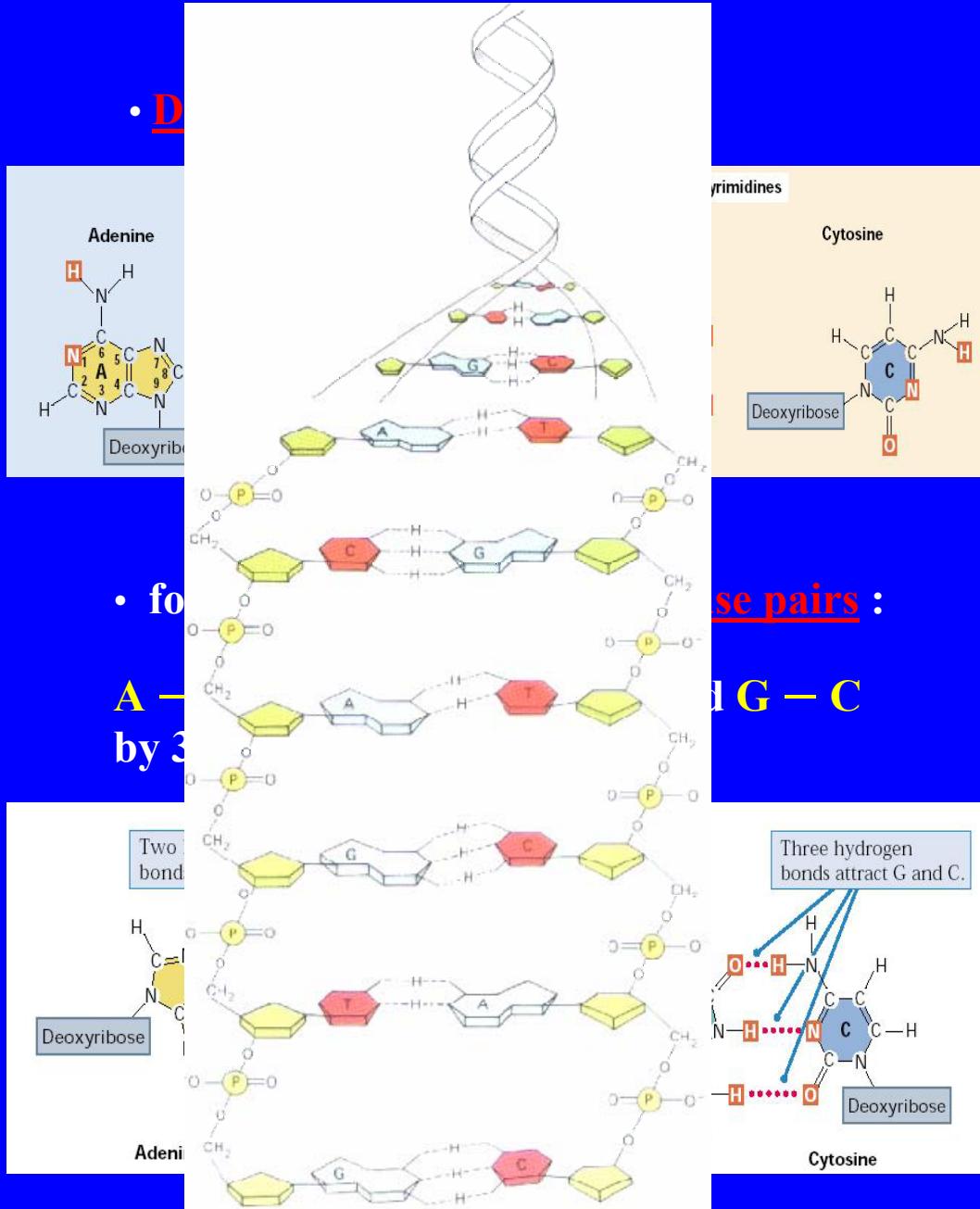
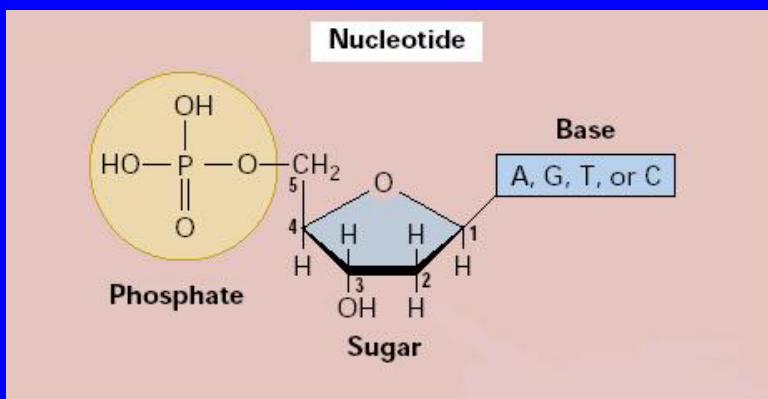


E. Braun et al, Nature 391, 775 (1998).

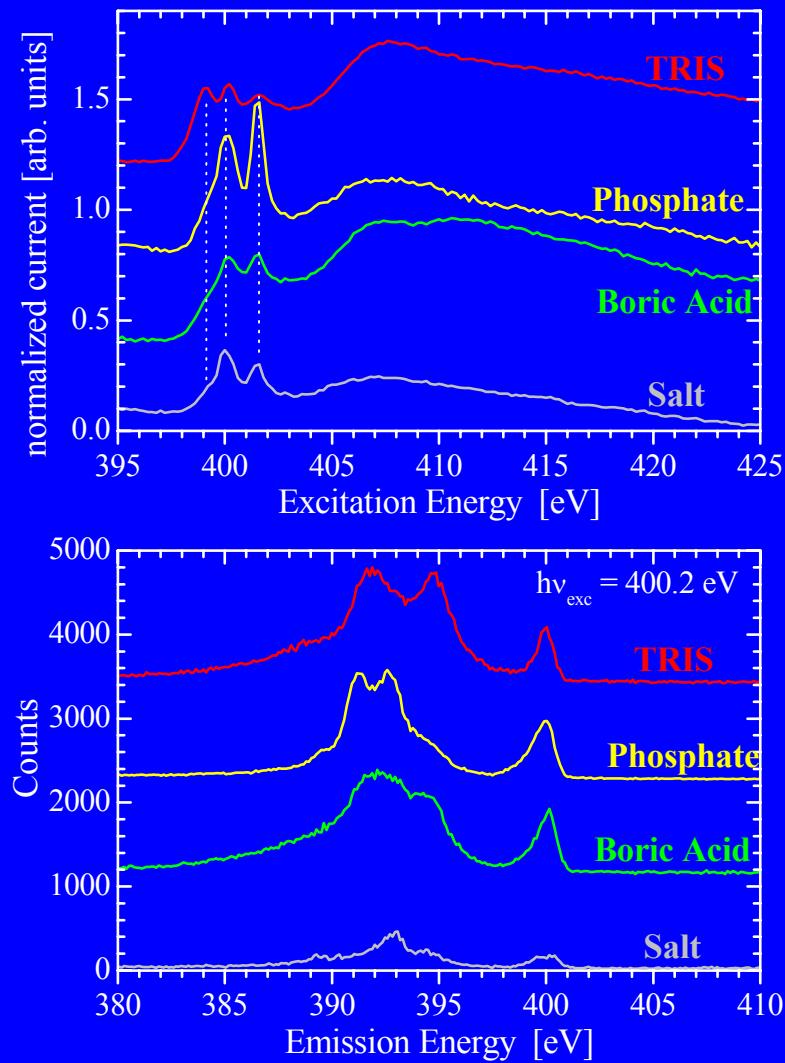
Great potential applications for DNA in Nanoelectronics
but is DNA a good conductor?

The electronic structure of DNA (Deoxyribonucleic Acid)

- Nucleic acids are polymers of nucleotides.
- A nucleotide consists of
 - a **nitrogenous base**,
 - a pentose sugar and
 - a **phosphate group**.
- Sugar – phosphate forms backbone.



The effect of the buffer materials for DNA



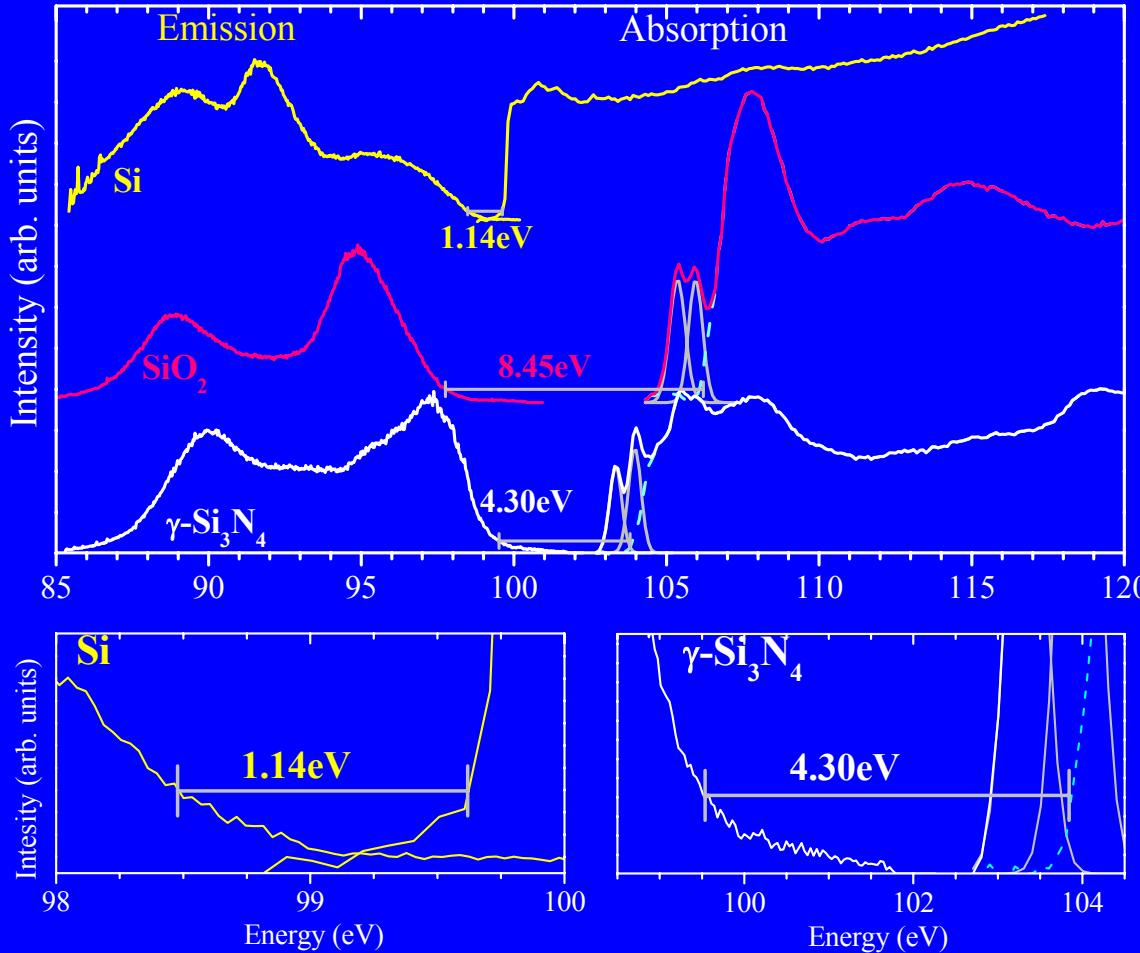
A. Moewes, J. MacNaughton, R. Wilks et al,
J. Electr. Spectr. 137, 817 (2004).

Choice of buffer material strongly affects the electronic structure of DNA.

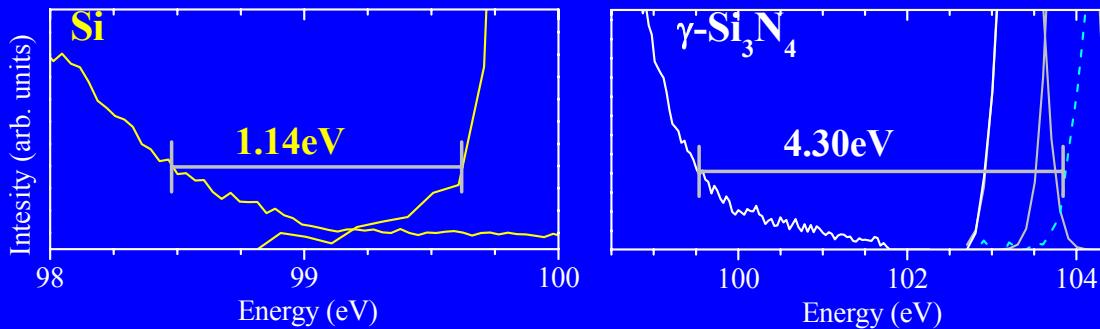
The band gap of $\gamma\text{-Si}_3\text{N}_4$

Problem: No single crystal available, band gap measurements are difficult.

Solution: Measure occupied (XES) and unoccupied (XAS) density of states:



S. Leitch, A. Moewes et al,
J. Phys. Cond. Matt. 16, 6469
(2004).



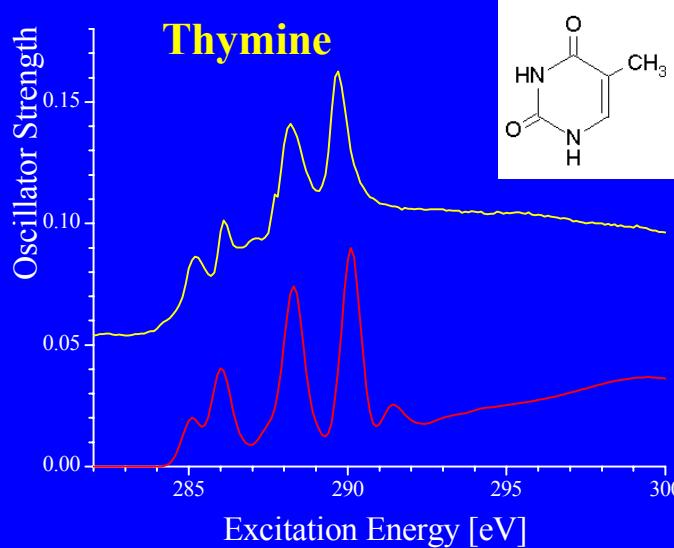
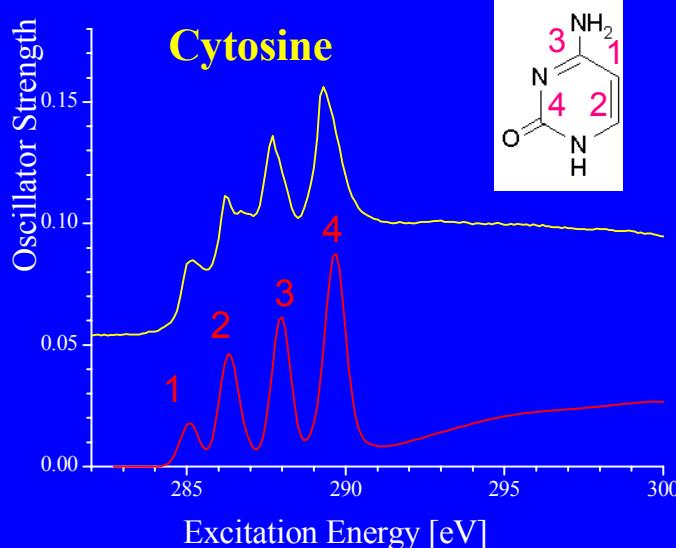
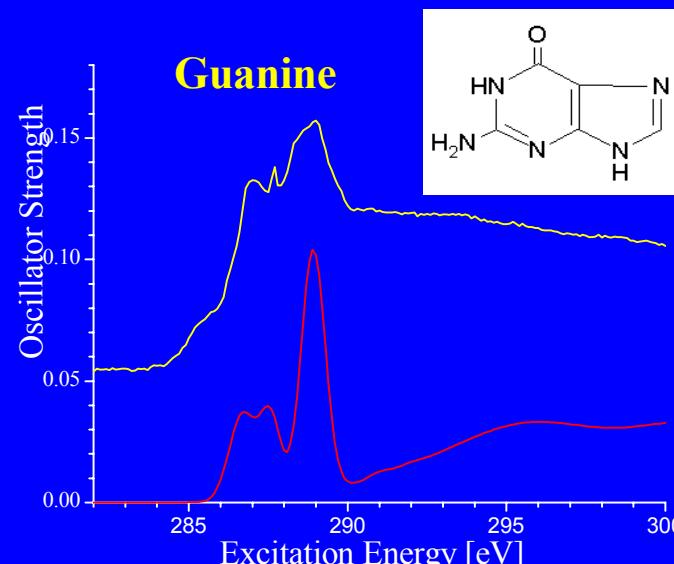
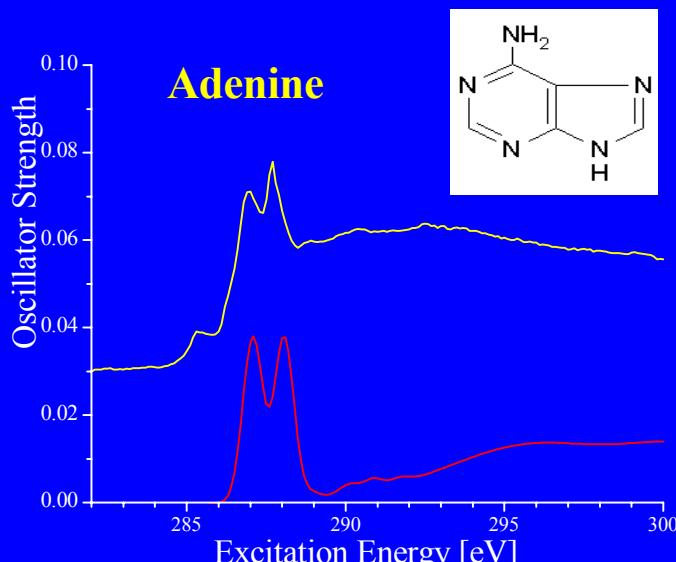
Without accounting for “exciton”, the band gap value would be 3.42 eV.

Our experimental determination of band gap for $\gamma\text{-Si}_3\text{N}_4$: 4.3 ± 0.25 eV

Theory: 3.45 eV [Mo PRL 83, 5046 (1999) and our calculations].

Only other experimental value (UV abs.): 3.3 eV [Zerr et al, Act. Crystallogr. 58, C47 (2002)].

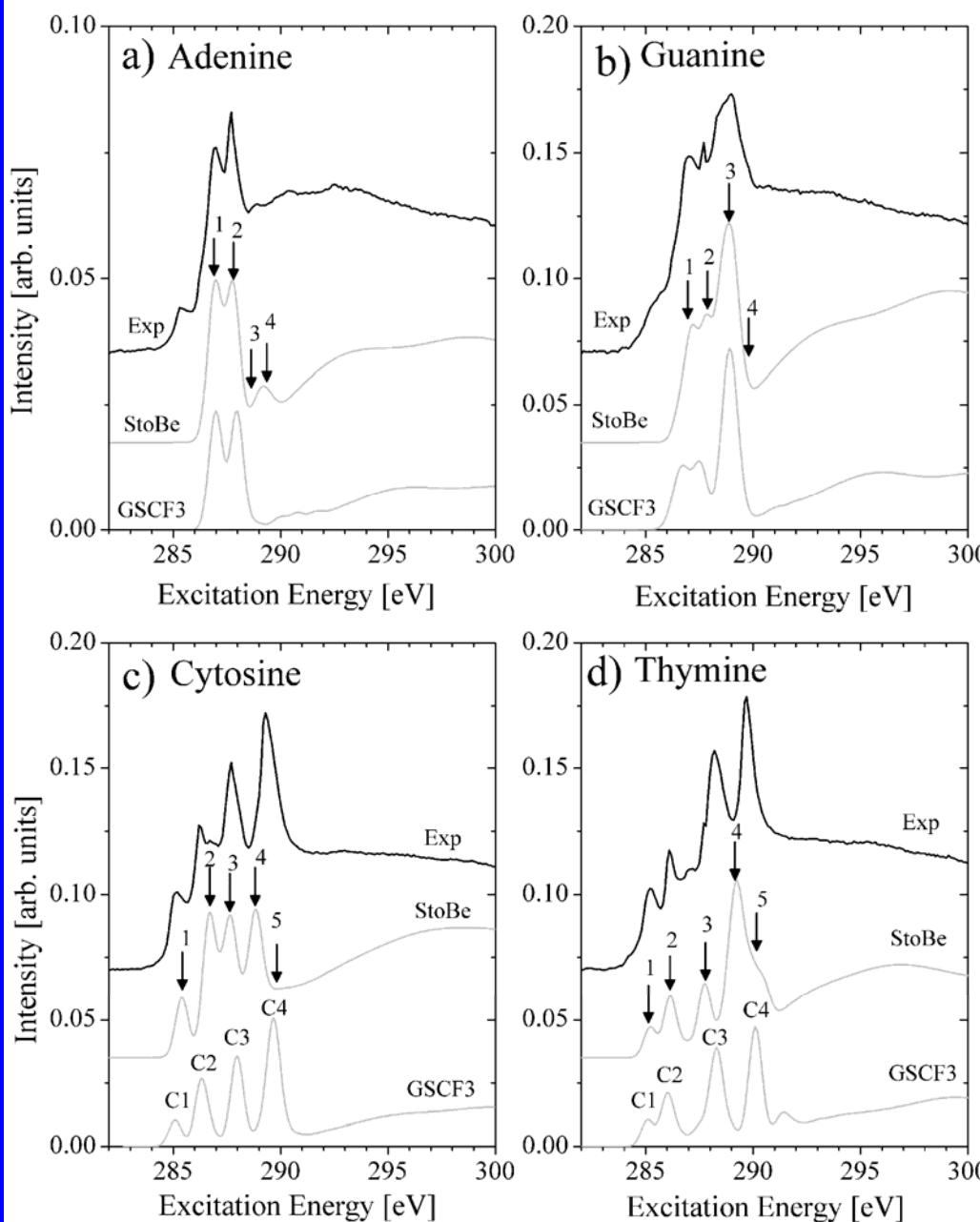
StoBe calculations for the DNA bases : C 1s XAS



J. MacNaughton, A. Moewes et al., J. Phys. Chem. B 109, 7749 (2005).

Excellent agreement between all C 1s XAS and H.-F. calculations.

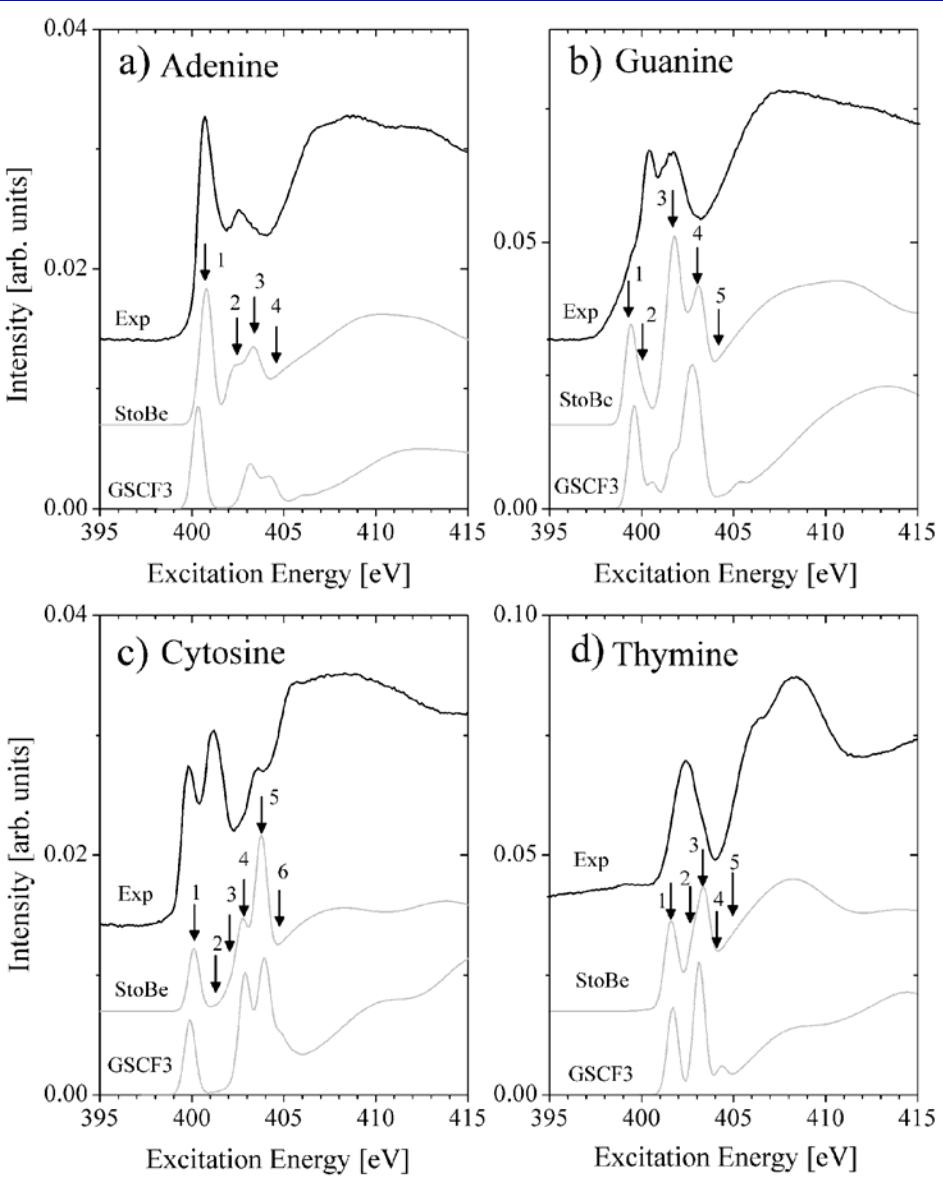
C 1s absorption of Nucleobases



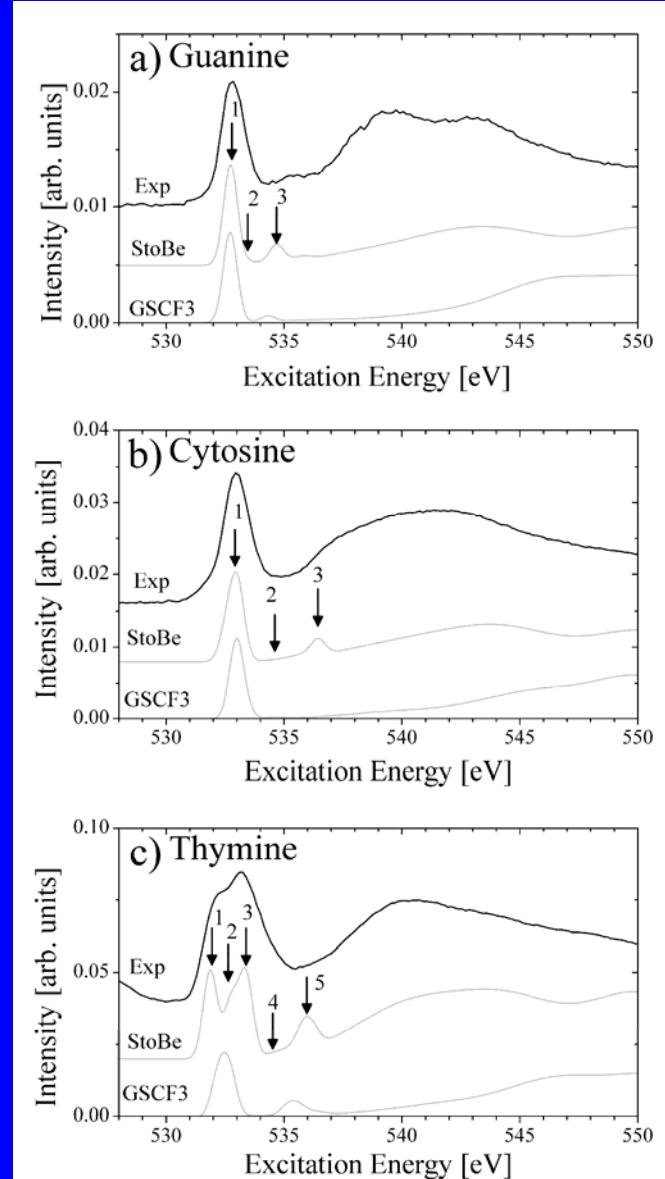
J. MacNaughton, A.
Moewes et al.,
J. Phys. Chem. B 109,
7749 (2005).

N and O absorption

N 1s XAS



O 1s XAS



Where do I see future improvements?

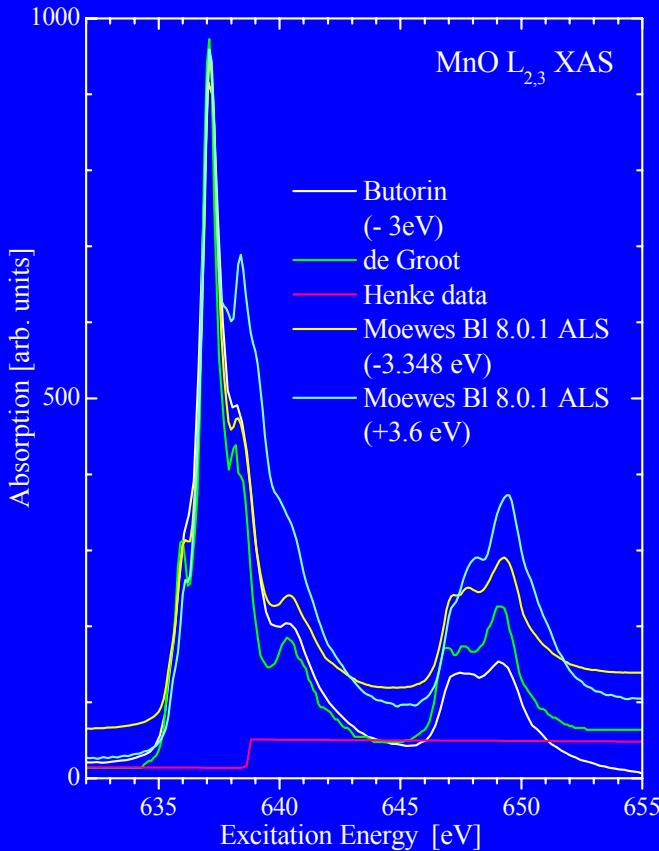
1. Obtain quantifiable spectra.

- Different beamlines...
- Transmission, TEY, PFY, TFY, Raman...

2. Complex materials in different phases

- liquid and solid
- under surface prep. conditions.

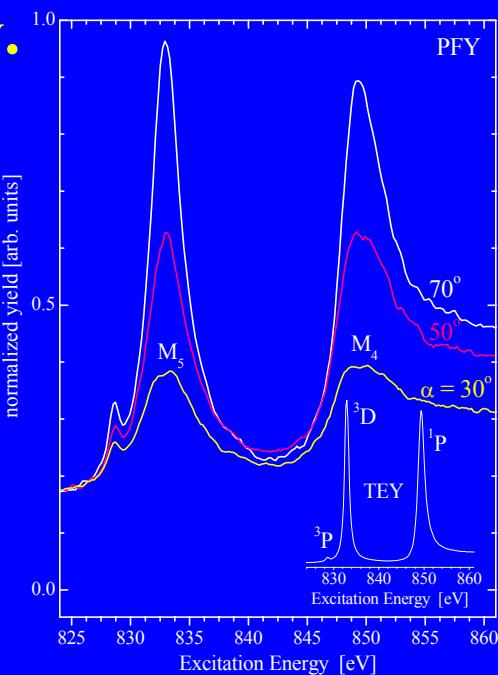
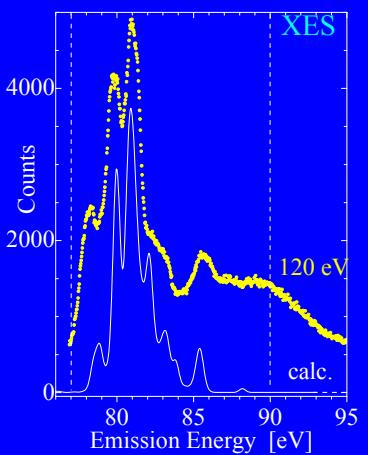
3. Avoid and understand radiation damage.



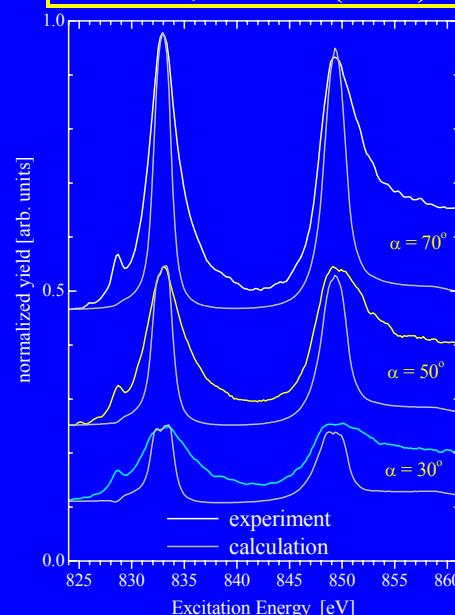
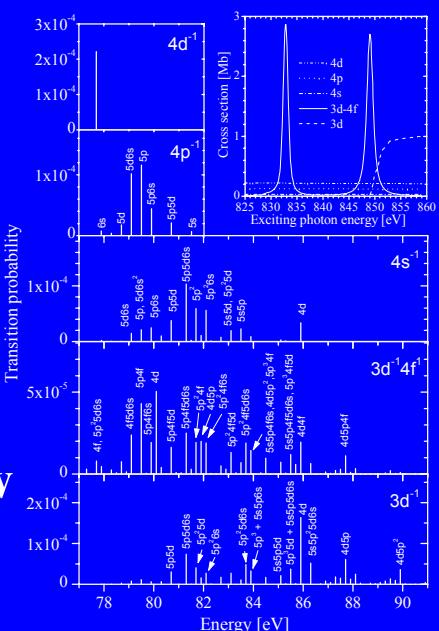
4. Understand multiple excitations and their decay.

What happens to (La) emission from a high-lying threshold ($5p \rightarrow 4d$ at 84 eV) when exciting at lower lying threshold ($3d \rightarrow 4f$ around 840 eV)?

- Cascade processes need to be taken into account and correction for self-absorption.
- Contrast agrees well for calc. and exp. but
- Integral exp. intensity is 2.4 times larger than for calculation.
- The emission spectra do not follow the expectations at all!!!

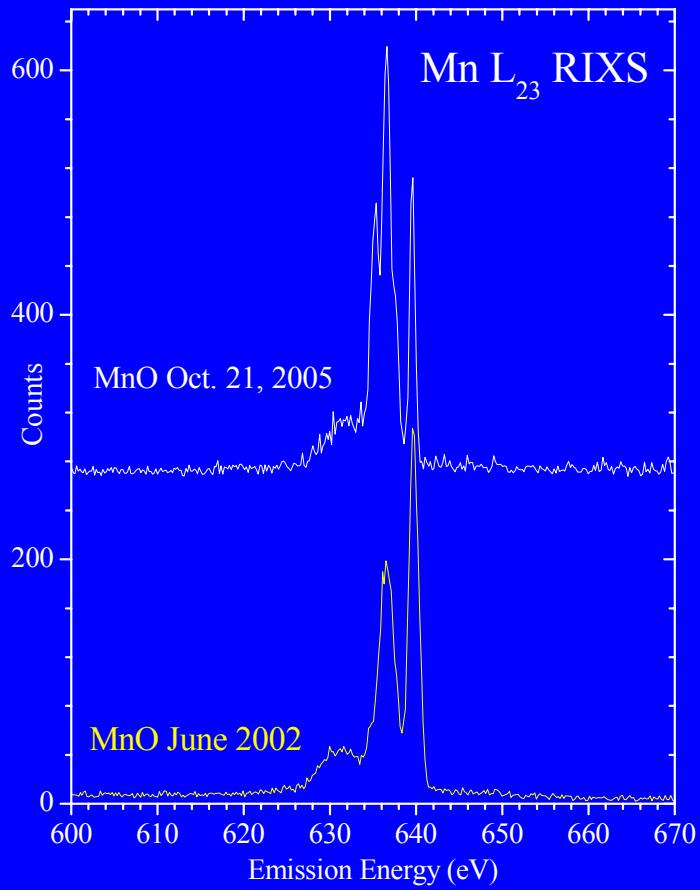


A. Moewes, R. Wilks
PRB 72, 075129 (2005)

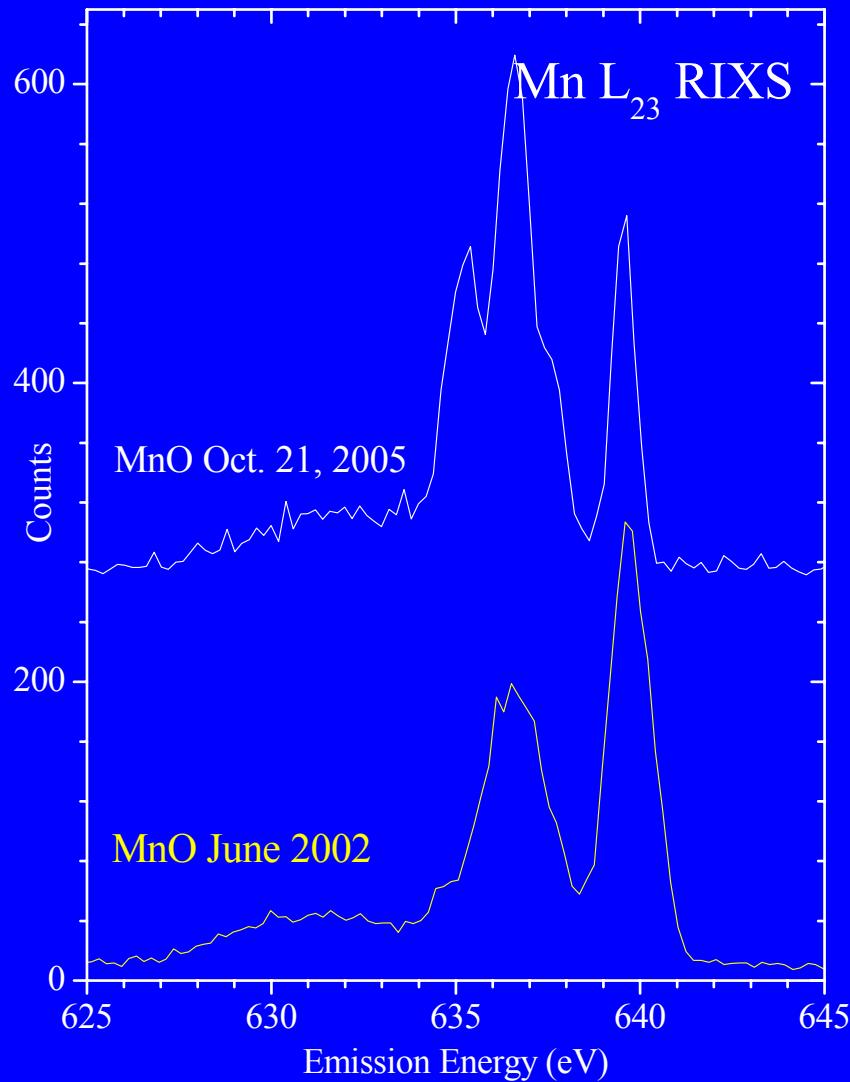


Acknowledgements

Thank you Jonathan!



0.37 eV FWHM at 640 eV.



Acknowledgements

Synthesis of B-DNA by

- J.S. Lee / U of S, Dept. of Biochemistry and
- H.-B. Kraatz / U of S, Dept. of Chemistry

Funding by

- NSERC 
- CFI 
- Canada Research Chair Program 
- U of S & Dept. of Physics (scholarships) 